molecule or molecular complex comprising a calcineurin A (CnA) binding pocket defined by structure coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 232, 253, 254, 256, 281, 282, 283, 284, 306, 311, 312, and 317 according to Figure 1, or a homologue of said molecule or molecular complex wherein said homologue comprises a CnA homologue binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å;

wherein said method comprises the steps of:

a. employing computational means to perform a fitting operation between the chemical entity and the CnA binding pocket or the CnA homologue binding pocket;

b. analyzing the results of said fitting operation to quantify the association between the chemical entity and the CnA binding pocket or the CnA homologue binding pocket; and

c. outputting said quantified association to a suitable output hardware.

20. (Twice amended) A method for evaluating the ability of a chemical entity to associate with a crystallized molecule or molecular complex comprising a CnA binding pocket defined by structure coordinates of CnA amino acids 90, 91,

92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 281, 282, 283, 306, 311, 232, and 254, according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a CnA homologue binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å;

wherein said method comprises the steps of:

a. employing computational means to perform a fitting operation between the chemical entity and the CnA binding pocket or the CnA homologue binding pocket;

b. analyzing the results of said fitting operation to quantify the association between the chemical entity and the CnA binding pocket or the CnA homologue binding pocket; and

c. outputting said quantified association to a suitable output hardware.

21. (Twice amended) A method for evaluating the ability of a chemical entity to associate with a crystallized molecule or molecular complex comprising a CnA/CnB binding pocket defined by structure coordinates of CnA amino acids 122, 124, 159, 160, 310, 312, 313, 314, 339, 341, 343, 344, 345, 347, 351, 352, 353, 354, 355, 356, 359, 360, and 363; and calcineurin B (CnB) amino acids 49, 50, 114, 115, 118,

119, 121, 122, 123, 124, 157, 158, 159, 161, and 162 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a CnA/CnB homologue binding pocket that has a root mean square deviation from the backbone atoms of said CnA and CnB amino acids of not more than 1.5Å;

wherein said method comprises the steps of:

a. employing computational means to perform a fitting operation between the chemical entity and the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket;

b. analyzing the results of said fitting operation to quantify the association between the chemical entity and the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket; and

c. outputting said quantified association to a suitable output hardware.

9 ~~22~~. (Twice amended) The method according to claim 7 ~~19~~ or 8 ~~20~~, wherein said crystallized molecule or molecular complex further comprises a second binding pocket defined by CnA amino acids 122, 124, 159, 160, 310, 312, 313, 314, 339, 341, 343, 344, 345, 347, 351, 352, 353, 354, 355, 356, 359, 360, and 363; and CnB amino acids 49, 50, 114, 115, 118, 119,

121, 122, 123, 124, 157, 158, 159, 161, and 162; according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a second homologue binding pocket that has a root mean square deviation from the backbone atoms of said CnA and CnB amino acids of not more than 1.5Å.

10 ~~23~~. (Twice Amended) The method according to claim 9 ~~22~~, wherein said crystallized molecule or molecular complex is defined by the entire set of structure coordinates according to Figure 1, or a homologue thereof, wherein said homologue has a root mean square deviation from the backbone atoms of said CnA and CnB amino acids of not more than 1.5Å.

11 ~~24~~. (Twice Amended) The method according to claim 9 ~~22~~, wherein said molecule or molecular complex comprises amino acids 17-392 of CnA, amino acids 1-169 of CnB, intact FKBP12 and FK506.

REMARKS

Applicants have amended claims 19-24 in response to the Examiner's objections and rejections (see below).

Specifically, applicants have amended claims 19 and 21 to recite an outputting step. Support for this amendment may